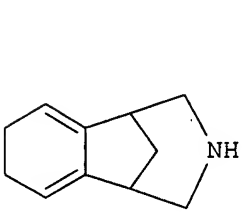
4/14/05

ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:462904 CAPLUS
DOCUMENT NUMBER: 141:190669
TITLE: Preparation of 1,5-Methano-2,3,4,5-tetrahydro-1H-3-benzazepine via Pd-Catalyzed Cyclization
AUTHOR(S): Singer, Robert A.; McKinley, Jason D.; Barbe, Guillaume; Farlow, Robin A.
CORPORATE SOURCE: Chemical Research and Development, Pfizer Global Research and Development, Pfizer Inc., Groton, CT, 06340, USA
SOURCE: Organic Letters (2004), 6(14), 2357-2360
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:190669
GI



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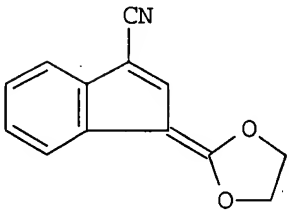

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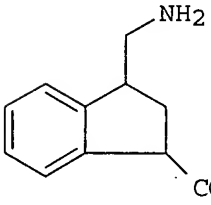

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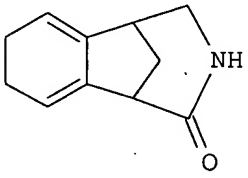
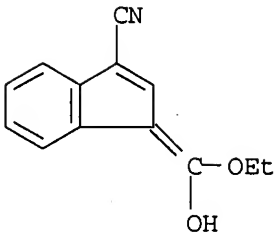


IV

AB A new approach to prepare 1,5-methano-2,3,4,5-tetrahydro-1H-3-benzanepine (I) is discussed. This strategy utilized a tandem Michael addition and Pd-catalyzed cyclization to afford cyanobenzofulvene acetal II. This indene intermediate (II) was subjected to hydrogenolysis to provide an amino ester (III) and was cyclized with base to afford lactam IV. The lactam (IV) was reduced with borane to afford the desired benzazepine (I).

IT **474024-31-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1,5-methano-2,3,4,5- tetrahydro-1H-3-benzazepine via tandem Michael addition and Pd-catalyzed indene cyclization, hydrogenolysis, lactam cyclization, and reduction)

RN 474024-31-2 CAPLUS
CN 1H-Indene-3-carbonitrile, 1-(ethoxyhydroxymethylene)-, sodium salt (9CI) (CA INDEX NAME)



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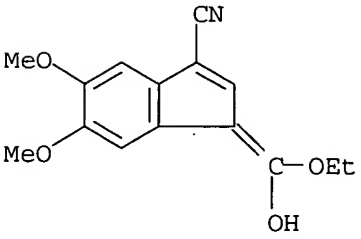
IT **474024-32-3P 474024-33-4P 474024-34-5P**
474024-35-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 1,5-methano-2,3,4,5- tetrahydro-1H-3-benzazepine via tandem Michael addition and Pd-catalyzed indene cyclization, hydrogenolysis, lactam cyclization, and reduction)

RN 474024-32-3 CAPLUS
CN 1H-Indene-3-carbonitrile, 1-(ethoxyhydroxymethylene)-5,6-dimethoxy-, sodium salt (9CI) (CA INDEX NAME)



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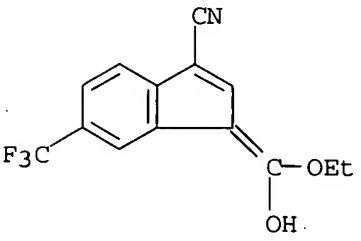
RN 474024-33-4 CAPLUS
CN 1H-Indene-3-carbonitrile, 1-(ethoxyhydroxymethylene)-6-(trifluoromethyl)-, sodium salt (9CI) (CA INDEX NAME)



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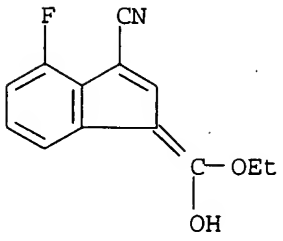
RN 474024-34-5 CAPLUS
CN 1H-Indene-3-carbonitrile, 1-(ethoxyhydroxymethylene)-4-fluoro-, sodium salt (9CI) (CA INDEX NAME)



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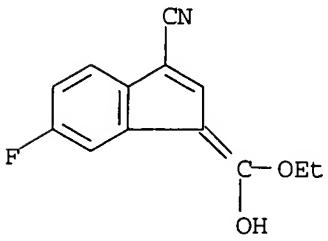
RN 474024-35-6 CAPLUS
CN 1H-Indene-3-carbonitrile, 1-(ethoxyhydroxymethylene)-6-fluoro-, sodium salt (9CI) (CA INDEX NAME)



● Na

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:832750 CAPLUS
DOCUMENT NUMBER: 137:337794
TITLE: Process for the preparation of 1,3-substituted indenes and aryl-fused azapolycyclic compounds
INVENTOR(S): Singer, Robert Alan; McKinley, Jason Daniel
PATENT ASSIGNEE(S): Pfizer Products Inc., USA
SOURCE: PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002085843	A2	20021031	WO 2002-IB660	20020304
WO 2002085843	A3	20030605		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA,

GN, GQ, GW, ML, MR, NE, SN, TD, TG

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EP 1383733	A2	20040128	EP 2002-701498		20020304
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BR 2002008992	A	20040427	BR 2002-8992		20020304
JP 2004527545	T2	20040909	JP 2002-583371		20020304
US 2003060624	A1	20030327	US 2002-124135		20020417
ZA 2003007205	A	20040915	ZA 2003-7205		20030915
PRIORITY APPLN. INFO.:			US 2001-285131P	P	20010420
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OTHER SOURCE(S): MARPAT 137:337794

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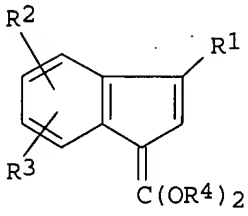

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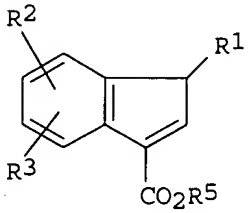

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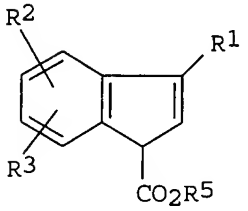

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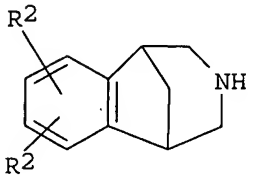


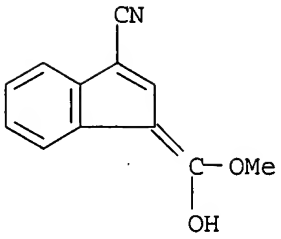
IV

AB The 1,3-substituted indenes I-III [R1 = CN, alkoxycarbonyl, acyl, aryl, NO2, CF3, sulfonyl; R2, R3 = H, F, Cl, alkylthio, alkylsulfinyl, alkylsulfonyl, (un)substituted NH2, CO2H, CONH2, SO2NH2, alkoxy etc.; R4 = H, ammonium, alkali metal; R5 = alkyl, trialkylsilyl, SiPh3] were prepared as intermediates for the benzoazabicyclooctanones IV which modulate cholinergic function. Thus, 2-BrC6H4CH2CN was treated with MeOCH:CHCO2Me to give 2-BrC6H4C(CN):CHCH2CO2Me which was cyclized to 3-(hydroxymethoxymethylene)-3H-indene-1-carbonitrile sodium salt. Reductive cyclization of the latter compound gave 2,3,4,5-tetrahydro-1,5-methano-1H-benzazepin-2-one.

IT **474024-30-1P 474024-31-2P 474024-40-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1,3-substituted indenes as intermediates for aryl-fused azapolycyclic compds. with cholinergic function)

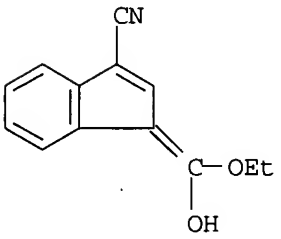
RN 474024-30-1 CAPLUS

CN 1H-Indene-3-carbonitrile, 1-(hydroxymethoxymethylene)-, sodium salt (9CI) (CA INDEX NAME)



● Na

RN 474024-31-2 CAPLUS
CN 1H-Indene-3-carbonitrile, 1-(ethoxyhydroxymethylene)-, sodium salt (9CI) (CA INDEX NAME)



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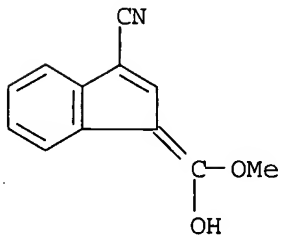
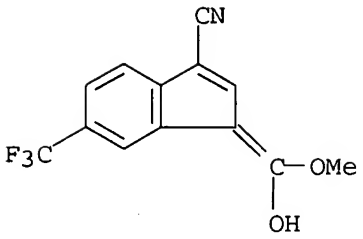
RN 474024-40-3 CAPLUS
CN 1H-Indene-3-carbonitrile, 1-(hydroxymethoxymethylene)- (9CI) (CA INDEX NAME)



IT **474024-28-7P 474024-32-3P 474024-33-4P**
474024-34-5P 474024-35-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 1,3-substituted indenes as intermediates for aryl-fused azapolycyclic compds. with cholinergic function)
RN 474024-28-7 CAPLUS
CN 1H-Indene-3-carbonitrile, 1-(hydroxymethoxymethylene)-6-(trifluoromethyl)-, sodium salt (9CI) (CA INDEX NAME)



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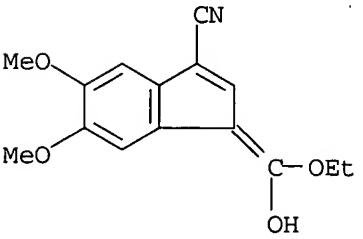

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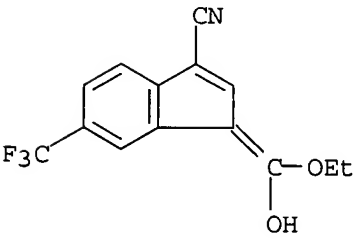

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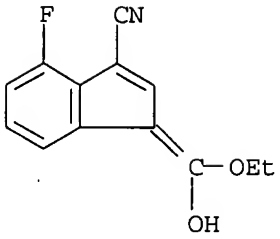
RN 474024-34-5 CAPLUS
CN 1H-Indene-3-carbonitrile, 1-(ethoxyhydroxymethylene)-4-fluoro-, sodium salt (9CI) (CA INDEX NAME)



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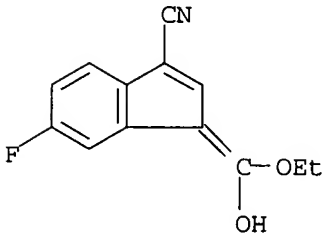
RN 474024-35-6 CAPLUS
CN 1H-Indene-3-carbonitrile, 1-(ethoxyhydroxymethylene)-6-fluoro-, sodium salt (9CI) (CA INDEX NAME)



● Na

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4/14/05

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Structure attributes must be viewed using STN Express query preparation.

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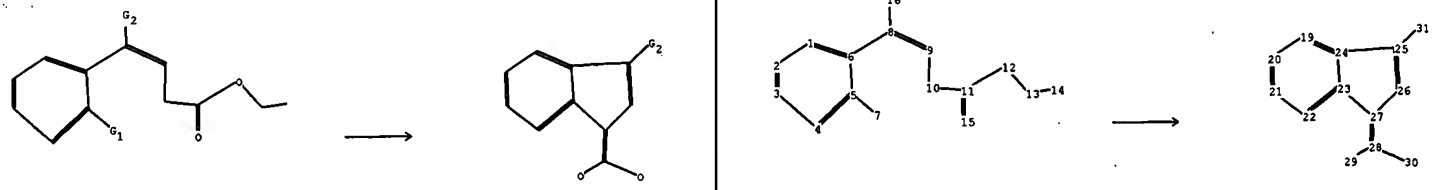

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ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 19-20 19-24 20-21 21-22 22-23 23-24 23-27 24-25
25-26 26-27
exact/norm bonds :
5-7 8-16 11-12 11-15 12-13 23-27 24-25 25-26 25-31 26-27 28-29 28-30
exact bonds :
6-8 8-9 9-10 10-11 13-14 27-28
normalized bonds :
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G1:Cl,Br,F,I

G2:Ph,CO2H,CN,OSO3H,C(O)CH3,NO2

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fragments assigned reactant/reagent role:
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4/14/05

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L1 HAS NO ANSWERS
L1              STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


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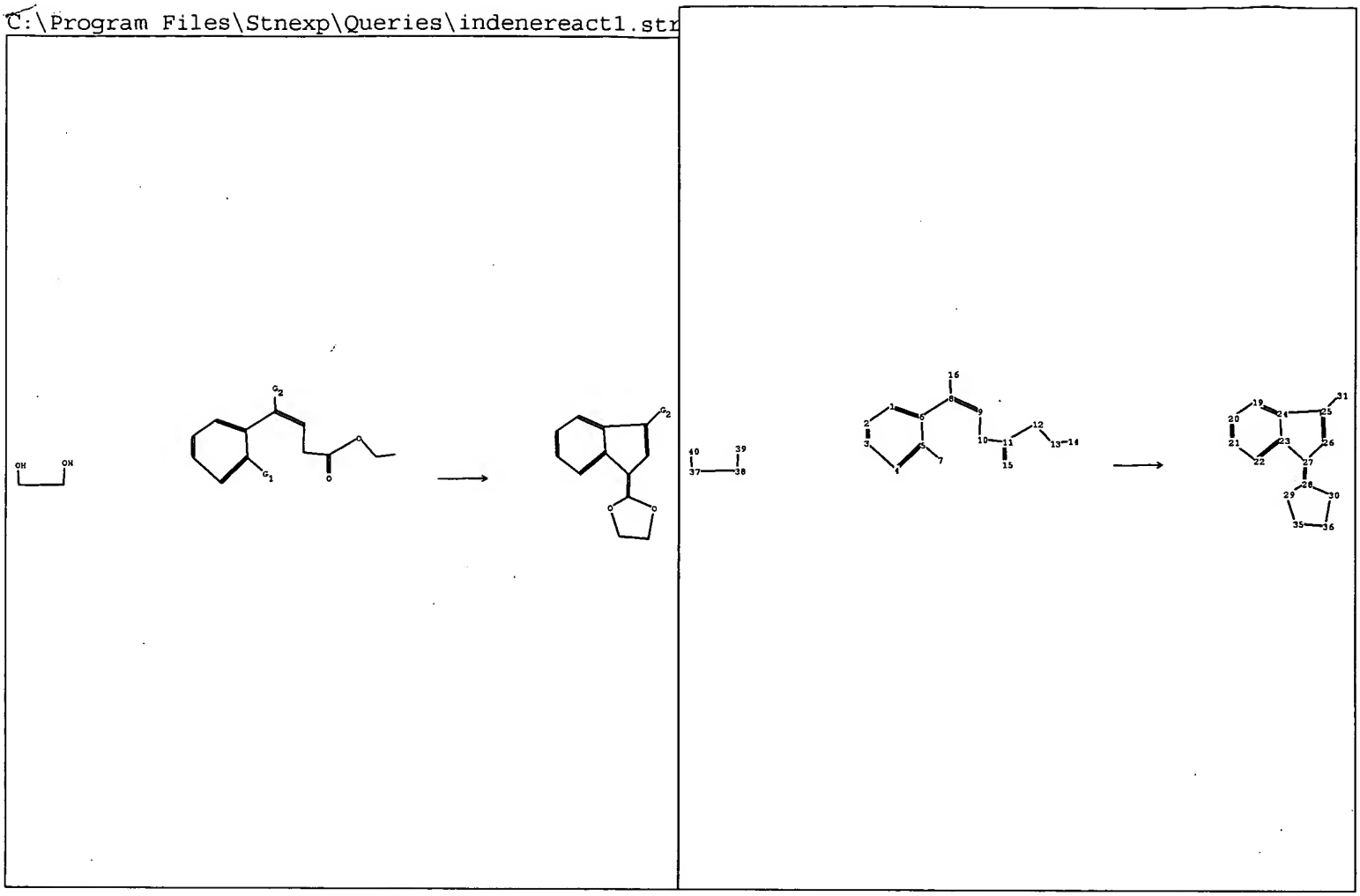

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ring nodes :
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ring bonds :
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25-26 26-27 28-29 28-30 29-35 30-36 35-36
exact/norm bonds :
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exact bonds :
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normalized bonds :
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G1:Cl,Br,F,I

G2:Ph,CO2H,CN,OSO3H,C(O)CH3,NO2

Match level :
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11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 19:Atom 20:Atom 21:Atom
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31:CLASS 35:Atom 36:Atom 37:CLASS 38:CLASS 39:CLASS 40:CLASS
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containing 37
fragments assigned product role: